

Network Null Model based on Maximal Entropy and the Rich–Club

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Abstract

We present a method to construct a network null-model based on the maximum entropy principle with the restrictions that the rich-club and the degree sequence are conserved. We show that the probability that two nodes share a link can be described with a simple mass probability function, which in turn, allow us to approximate the maximum entropy solution for large networks. As an example, we evaluate the null-model of three real networks and show that the average degree-degree correlation is well approximated by the null.

1 Introduction

Information measures based on Shannon’s entropy are used to characterise the complexity of networks [1, 2, 3]. Shannon’s entropy can also be used to obtain the network ensemble that best describes our state of knowledge of the network structure. In this case the maximal entropy approach (MAXENT) is used to describe our state of knowledge in a way that is “maximally noncommittal” by certain criterion [4]. The MAXENT solutions represent the best predictions we are able to make based on the given information. Maximising the entropy defines a network ensemble that can be considered as a null-model of the network under certain structural constraints. The null-model is used to make inferences in networks problems.

Recently, using entropic measure, Bianconi [2, 5] has formulated how to evaluate different network ensembles that conserve different structural constraints like the degree sequence, the average degree-degree distribution and the community structure. More recently Johnson et. al [6] using the MAXENT approach, obtained that for a scale-free network defined only by their degree sequence the most likely structure of the networks, the null-model, is to be disassortative. Their result was obtained using the ansatz that the average degree-degree correlation of the network can be described with a power law.

Here, using MAXENT, we construct an ensemble of networks that is defined by the rich-club coefficient and the degree sequence. There are several reasons why we impose these network restrictions. In scale-free networks [7] the connectivity of the rich-club plays an important role in the functionality of the network [8], for example in the transmission of rumours in social networks [9], the efficient delivery of information in the Internet [10] and the organisation of the human brain connectivity [11]. Also, the approach to describe a network using the average degree-degree correlation has been criticised as it could be ambiguous when classifying the assortativity of a network [8]. The rich-club coefficient does not suffer from these disadvantages and it is also related to the degree-degree correlation [12]. Finally, recently we introduced a method to build surrogate networks based on the conservation of the degree sequence and rich-club coefficient [13]. We would like to know if the surrogates are biased.

Section 2 gives a brief background of how to construct surrogates networks that conserve the rank based rich-club coefficient. Section 3 evaluates the MAXENT solution for network ensembles generated by conserving the rich-club coefficient and degree sequence. We provide a formula to evaluate the mass probability function describing the node node connectivity. In section 4 we show some of examples, based on real networks, on how to evaluate the MAXENT solution and relate some properties of this solution with the structure of the network. We also show how to approximate the MAXENT solution for large networks. Section 5 contains our conclusions.

2 Surrogates that conserve the rich-club coefficient

If the nodes are ranked in decreasing order of their degree, first node has the highest degree, second node the second highest degree and so on, we can characterise the network connectivity using the node's degree k_r and the number of links $\Delta E(r)$ that node r shares with nodes of higher degree. In other words $\Delta E(r)$ is the number of links that node r shares with the nodes $r \in [1, r-1]$. The total number of links is $L = \sum_{i=1}^N \Delta E(i)$ and the rich-club coefficient [14] is

$$\Phi(r) = \frac{2}{r(r-1)} \sum_{i=1}^r \Delta E(i), \quad (1)$$

which is the density of links between the top r ranked nodes. It is possible to generate a surrogate network that conserves $\Delta E(r)$ for all r , which is equivalent to conserve the rich-club $\Phi(r)$. Let us assume that $P(r', r)$ is the probability that node r connects to node r' and that $P(r, r) = 0$ as self-loops are not allowed. Given the $\Delta E(r)$ links, we constrain the connectivity of a network by imposing the condition that the average number of links, $\overline{\Delta E}(r)$ satisfies

$$\overline{\Delta E}(r) = \sum_{i=1}^{r-1} P(i, r) = \Delta E(r). \quad (2)$$

Under this condition the average degree \bar{k}_r of node r is

$$\bar{k}_r = \sum_{r'=1}^N P(r', r) = \Delta E(r) + \sum_{j=r+1}^N P(r, j) \quad (3)$$

with standard deviation $\sigma_{k_r}^2 = \sum_{r'=1}^N P(r', r)(1 - P(r', r))$. The average degree of the nearest-neighbours [15] of a node with degree k is

$$k_{nn}(k) = \sum_{k'=1}^{k_{\max}} k' P(k'|k) \approx \frac{1}{N_k} \sum_{i=1}^N \left(\frac{1}{k} \sum_{j=1}^N P(i, j) k_j \right) \delta_{k_i, k}, \quad (4)$$

where the Kronecker delta is introduced to consider only nodes with degree equal to k , N_k is the number of k -degree nodes and the term $1/k$ is a normalisation factor.

Previously [13] we proposed that the probability can be factorized as $P(r', r) = T(r', r) \Delta E(r)$, where $r' < r$ and $T(r', r)$ is a linking term. The simplest case is when the $\Delta E(r)$ links are evenly distributed between node r and the $r' < r$ nodes, then the probability that node r connects to r' is

$$P(r', r) = T(r', r) \Delta E(r) = \frac{1}{r-1} \Delta E(r), \quad r' < r, \quad (5)$$

where $T(r', r) = 1/(r-1)$. We called this the egalitarian case.

For the case that node r prefers to connect to nodes with lower rank (i.e. higher degree), we proposed the preferential linking term $T(r', r) = r'^{-\alpha}/S(r)$, where $\alpha > 0$ is a constant and $S(r)$ is a normalisation factor. The probability that there is a link between r and r' is

$$P(r', r) = \frac{r'^{-\alpha}}{S(r)} \Delta E(r) = \left(\frac{r'^{-\alpha}}{\sum_{i=1}^{r-1} i^{-\alpha}} \right) \Delta E(r), \quad (6)$$

where $S(r) = \sum_{i=1}^{r-1} i^{-\alpha}$ to ensure that $\sum_{i=1}^{r-1} P(i, r) = \Delta E(r)$.

3 Maximal Entropy

First we change the notation by using the label of the links to describe the probability that node i links with node j , that is $p_r = p_{g(i,j)}$ where $g(i, j)$ maps the labels of node i and j with the label r of the link that joins them. We assume that the network is undirected, has no self-loops, but allow that two nodes can share more than one link. Following the notation used in [16] the entropy

$$H(p_1, \dots, p_{N(N-1)/2}) = - \sum_{m=1}^{N(N-1)/2} p_m \log p_m \quad (7)$$

is maximised under the constraints that the probabilities p_r are normalised, i.e. $\sum_{r=1}^{N(N-1)/2} p_r = 1$, and the rich-club connectivity and the degree sequence are conserved. The normalisation condition can be satisfied if we notice that the total number of links in the network is $L = \sum_r \sum_{r'} P(r', r)$, so we consider the probability $p_{g(i,j)} = P(i, j)/L$. Using the transformation $p_m = \exp(-q_m)$ the constraints become $\sum_{r=1}^{N(N-1)/2} e^{-q_r} = 1$ and

$$\sum_{i=1}^{N(N-1)/2} f_r(i) e^{-q_i} = m_r, \quad r = 1, \dots, M \quad (8)$$

where m_r are M constraints that are related to q_i via the map $f_r(i)$. If the Lagrangian multipliers are $\lambda_0, \dots, \lambda_M$ then the partition function is

$$Z(\lambda_1, \lambda_2, \dots, \lambda_M) = e^{-1} \sum_{i=1}^{N(N-1)/2} e^{\sum_{j=1}^M \lambda_j f_j(i)} \quad (9)$$

where $\lambda_0 = -\log Z(\lambda_1, \dots, \lambda_M)$ and $m_r = \partial(\log Z(\lambda_1, \dots, \lambda_M))/\partial \lambda_r$. These partial derivatives are used to construct a set of M non-linear equations

$$\sum_{i=1}^{N(N-1)/2} (m_r - f_r(i)) e^{\sum_{j=1}^M \lambda_j f_j(i)} = 0, \quad r = 1, 2, \dots, M. \quad (10)$$

If we substitute $t_j = e^{\lambda_j}$ then Eq. (10) becomes

$$\sum_{i=1}^{N(N-1)/2} (m_r - f_r(i)) \prod_{j=1}^M t_j^{f_j(i)} = 0, \quad r = 1, 2, \dots, M. \quad (11)$$

and

$$\lambda_0 = 1 - \log \left(\sum_{i=1}^{N(N-1)/2} \prod_{j=1}^M t_j^{f_j(i)} \right) \quad (12)$$

From the above two equations the MAXENT solutions are

$$q_i = 1 - \lambda_0 - \sum_{r=1}^M \lambda_r f_r(i), \quad r = 1, 2, \dots, N(N-1)/2 \quad (13)$$

and $p_r = -\log(q_r)$.

3.1 Conserving the rich-club

To conserve only the rich-club connectivity, the constraints in eq. (8) are

$$\sum_{i=1}^{r-1} p_{g(i,r)} = \frac{\Delta E(r)}{L}. \quad (14)$$

where the condition $\Delta E(r)/L$ is to satisfy that the probabilities p_r are normalised. These constraints can be rewritten as

$$\sum_{i=1}^N h(i, r+1) p_{g(i, r+1)} = m_r, \quad r = 1, 2, \dots, N-1 \quad (15)$$

where $m_r = \Delta E(r)/L$ and

$$h(i, j) = \begin{cases} 1 & i < j \\ 0 & \text{otherwise.} \end{cases} \quad (16)$$

By using the properties of the $h(i, j)$ function, $p_{g(i, r+1)} = \exp(-q_{g(i, r+1)})$ and $t_j = e^{\lambda_j}$, Eq. (11) becomes the set of linear equations

$$r(m_r - 1)t_r + \sum_{i=1, i \neq r}^M i(m_r t_i) = 0, \quad r = 1, \dots, M. \quad (17)$$

Notice that if $m_r = 0$ then we have the trivial solution $t_r = 0$. From Eq. (13) the probabilities are $p_{g(i, j)} = e^{1-\lambda_0-\lambda_{j-1}}$, and if we take into consideration that the rich-club is conserved

$$\sum_{i=1}^{r-1} p_{g(i, r)} = \sum_{i=1}^{r-1} e^{1-\lambda_0-\lambda_{r-1}} = (r-1)e^{1-\lambda_0-\lambda_{r-1}} = \frac{\Delta E(r)}{L}, \quad (18)$$

which implies $e^{1-\lambda_0-\lambda_{r-1}} = \Delta E(r)/((r-1)L)$ then

$$p_{g(i, r)} = \frac{\Delta E(r)}{(r-1)L}, \quad i < r. \quad (19)$$

Showing that the egalitarian case described in Eq. (5) is a solution of the maximal entropy ensemble.

3.2 Conserving the rich-club and degree sequence

To conserve both the rich-club connectivity and degree sequence we use the constraint given by Eq. (14) plus the restriction that the degree sequence is conserved, which is given by

$$\sum_{i=r+1}^N p_{g(r, i)} = \frac{k_r - \Delta E(r)}{L}, \quad r = 1, \dots, N \quad (20)$$

and can be written as

$$\sum_{i=1}^N h(r, i) q_{g(r,1)} = m_{N-1+r}, \quad r = 1, 2, \dots, N-1 \quad (21)$$

where $m_{N-1+r} = (k_r - \Delta E(r))/L$. We can interpret Eqs. (14) and (21) as the condition that given node r , its links are explicitly divided into the ones that connect with nodes of higher degree ($\Delta E(r)$) and the ones that connect with nodes of lower degree ($k_r - \Delta E(r)$). Again by manipulating the constraints we have that Eq. (11) becomes the set of non-linear equations

$$\sum_{j=1}^{N-1} \left(\sum_{i=j}^{N-1} (m_r - \delta(i, r)) t_i \right) t_{N-1+j} = 0, \quad r < N-1 \quad (22)$$

and Eq. (21)

$$\sum_{j=1}^{N-1} \left(\sum_{i=j}^{N-1} (m_r - \delta(N-1+j, r)) t_i \right) t_{N-1+j} = 0, \quad N-1 < r \quad (23)$$

where $\delta(i, j)$ is the Kronecker delta.

From $q_i = 1 - \lambda_0 - \sum_{r=1}^M \lambda_r f_r(i)$, the MAXENT probabilities are $p_{g(i,j)} = e^{1-\lambda_0-\lambda_{j-1}} e^{-\lambda_{N+i}}$. The conservation of the rich-club implies that

$$\sum_{i=1}^{j-1} p_{g(i,j)} = e^{1-\lambda_0-\lambda_{j-1}} \sum_{i=1}^{j-1} e^{-\lambda_{N+i}} = \frac{\Delta E(j)}{L} \quad (24)$$

If we define the function $w(i) = e^{-\lambda_{N+i}}$ then the probability mass function can be written as

$$p_{g(i,j)} = \left(\frac{w(i)}{\sum_{m=1}^{j-1} w(m)} \right) \frac{\Delta E(j)}{L} = T(i, j) \frac{\Delta E(j)}{L}, \quad i < j \leq N, \quad (25)$$

where $e^{1-\lambda_0-\lambda_{j-1}} = \Delta E(j)/L$ and $T(i, j) = w(i) / \sum_{m=1}^{j-1} w(m)$.

Notice that if the function $w(i)$ for $i = 1, \dots, N$ is known then we can describe the probability of connection between all the nodes in the network. Knowing the functional form of $w(i)$ is equivalent, up to a constant factor, to knowing $T(i, N)$ for $i = 1, \dots, N$.

4 Examples

To study the properties of the linking term $T(i, N)$ and how it relates to the network structure we evaluated numerically the MAXENT solution for the following real networks.

4.1 Complex Network co-authorship

The network data is the giant component of the scientists working in the field of Complex Networks as collected by Newman [17]. In here, we consider the network as unweighted and undirected. This network has some characteristics that are interesting in our context. From the average degree-degree correlation the network cannot be classified as assortative or disassortative (Fig. 1(a)). The nodes of degree one do not share any links with nodes of degree two.

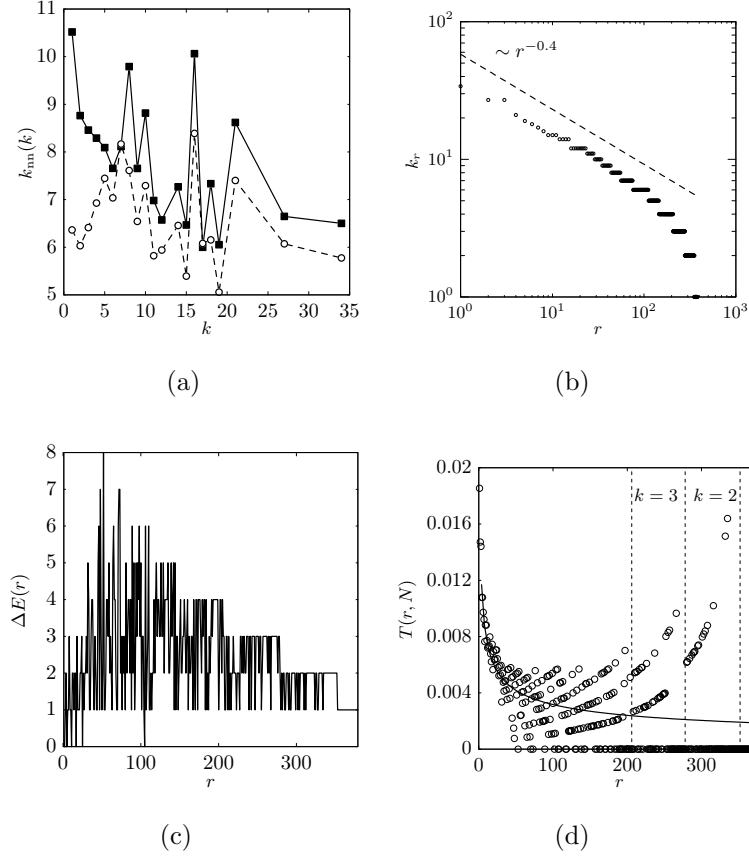


Figure 1: Co-authorship network. (a) Average degree-degree correlation (close-square data, open-circle MAXENT solution), (b) degree sequence, (c) number of links $\Delta E(r)$ share between node r and nodes $r' < r$ and (d) the linking term $T(r, N)$ obtained from the MAXENT solution. The network has 379 nodes and 916 links.

There is a tendency of nodes of similar low degree to connect with each other. This is expected as by construction all the co-authors of a paper are represented by a clique, that is if there is an article with four authors, the degree of these nodes is at least four and all these nodes are inter-connected. We use these properties of the network as a comparison point with the MAXENT solution. Figure 1(b) shows the degree sequence which, for small r , decays like a power law, and (c) the number of links $\Delta E(r)$ between node r and nodes $r' \in [1, r - 1]$. The nodes are ranked in decreasing order of their degree.

Figure 1(d) shows $T(r, N)$ obtained from the numerical solution of MAXENT. As previously mentioned in Eq. (25), this function describes the mass density function. We noticed that for small values of the rank, $T(r, N)$ decays in a similar fashion as the degree sequence. In this case proportional to $r^{-0.4}$ shown as a solid line in Fig 1(d). This reflects the property that there is a preferential attachment between the top ranked nodes.

As the value of r increases $T(r, N)$ decreases and around $r > 40$ increases again and has a “stepped” shape. The increment as r tends to N , shows that there is a preferential attachment between the low ranking nodes. The MAXENT solution captures the property that there is a tendency of low degree nodes to connect with low degree nodes. This reflects the property that there are papers with small number of authors that form cliques.

The MAXENT solution also reproduces the behaviour of the average degree-degree correlation $k_{nn}(k)$ which is shown in Fig 1(a) (open circles). For small k the discrepancy between the data and the MAXENT solution is because the MAXENT solution predicts that nodes with degree

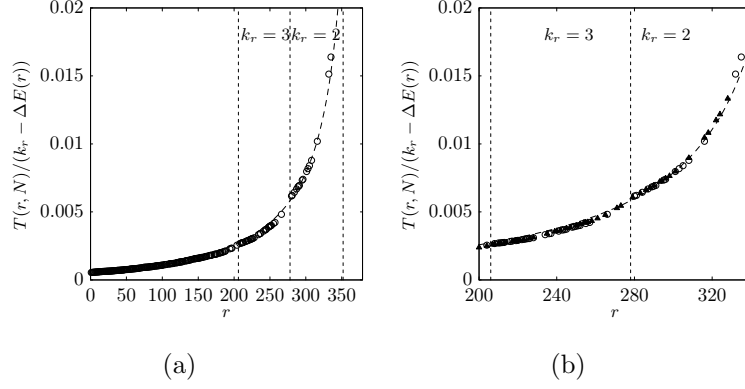


Figure 2: Co-authorship network. (a) Smoothing of the linking term $T(r, N)$, (b) The smooth linking term obtained using two different ranking schemes showed as open-circles and solid-triangles.

one and degree two should share some links. These kind of links are not present in the network data.

To understand the stepped behaviour of $T(r, N)$ we have marked in Fig. 1(d) with dashed lines the value of r where the degree of the nodes changes. The first observation is that if k_r is the degree of node r and $\Delta E(r)$ is the number of links that connect to nodes of higher rank, then $k_r - \Delta E(r)$ is the number of links that connect to nodes of lower rank. If $k_r - \Delta E(r) = 0$ means that a node $r' > r$ does not share a link with r . In other words, $T(r, N) = 0$ if $k_r - \Delta E(r) = 0$ which are the zeros shown in Fig. 1(d).

The second observation can be explained using the case $k_r = 3$ marked in Fig. 1(d). Consider the case that $k_r = 3$ where $k_r - \Delta E(r) = i$ and $i > 0$. if $i = 1$ means that from the possible three links that node r has, only one link connects to nodes with rank $r' > r$, we denote the probability of this happening as p . Now if $i = 2$ then there are two links that can connect node r' and r . If the MAXENT solution is non-bias then the probability that node r connects with r' is $p + p$, that is the probability that one of the free links connects the two nodes plus the probability that the other free link connects the two nodes. In Fig. 1(d), when $k_r = 3$, the case $k_r - \Delta E(r) = 1$ correspond to the lower step and $k_r - \Delta E(r) = 2$ to the upper step. The implication of this observation is that we can describe $T(r, N)$ via a non-stepped function. If we introduce the function $s(r) = T(r, N)/(k_r - \Delta E(r))$ where $k_r - \Delta E(r) \neq 0$ this function lies on a smooth curve, see Fig. 2(a).

The third observation obtained when fitting $s(r)$ to the data using least square is that $s(r)$ can be approximated well via $A/(N - r) + B$, where A and B are parameters. Partially we can justify this observation by noticing that if there are $N - r$ possible nodes where a link can be attached to, then the un-bias probability that we attach this link to any of these nodes is proportional to $1/(N - r)$.

Our final observation is that the MAXENT solution depends on the way that the nodes are ranked. There is an ambiguity when labelling the nodes via a degree-dependent rank. For high degree nodes this is not a problem, as the degree tend to be unique so the rank labels these nodes unambiguously. For lower degree nodes, there are many nodes with the same degree. In this case the labelling of the nodes is not unique. However when we evaluated the MAXENT solution using different ranking schemes for the nodes with equal degree, we noticed that the behaviour of $s(r)$ is independent of the ranking scheme, see Fig. 2(b).

Putting these observations together with Eq. (25) implies that the probability that node i is

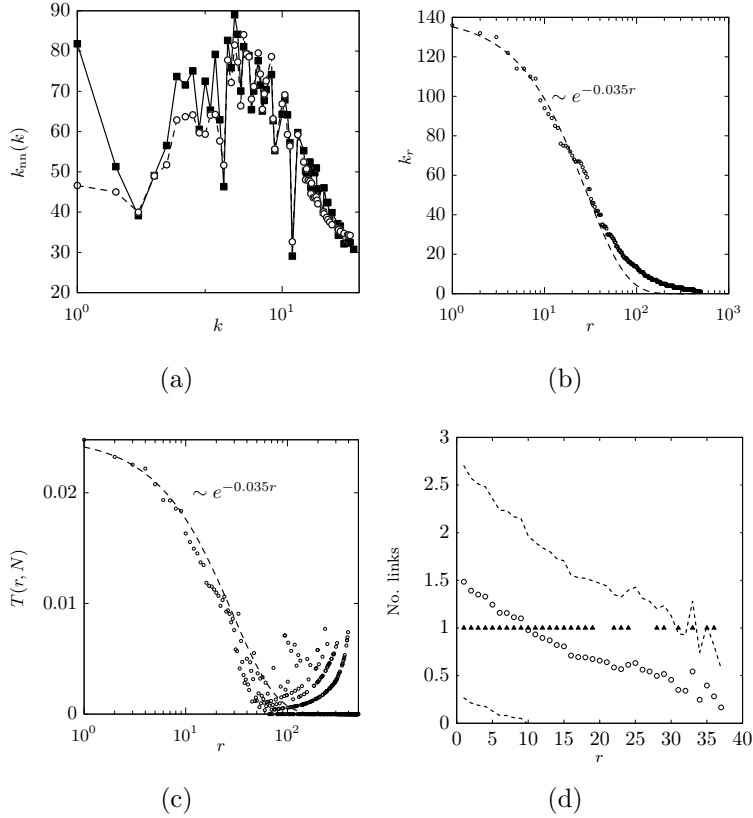


Figure 3: Airports Network. (a) Average degree–degree correlation of the airports network (solid square) and the null model (open circle) from the MAXENT solution. (b) The degree sequence which decays exponentially fast for small values of r . (c) Linking term $T(r, N)$ which for small r decays similarly as the degree sequence. (d) The links between the first 37 nodes and node 38 are marked with a solid triangle. Average number of links obtained from the null–model (open circle) and its standard deviation (dotted lines).

connected to node j is of the form

$$p_{g(i,j)} = \begin{cases} \frac{s(i)(k_i - \Delta E(i))}{\sum_{n=1}^{j-1} s(n)(k_n - \Delta E(n))} \left(\frac{\Delta E(j)}{L} \right) & i < j \\ 0 & \text{otherwise} \end{cases} \quad (26)$$

where $s(i) \sim A/(N - i) + B$. This is the main result of this paper.

4.2 Airports

In the US air transportation network the nodes are airports and an edge represents a direct flight between the two airports [18]. Fig. 3(a) shows that the average degree–degree correlation of the network (solid squares) is well approximated with the MAXENT solution (open circles). Again as in the case seen in the co–authorship network the MAXENT predicts more links between nodes of low degree. This is also clear in Fig. 3(c), which shows that high values of r (low degree) the probability of connection increases. Also notice that as the case of the co–authors network, the $T(r, N)$ behaves similarly as the degree distribution for small r .

We are interested in this network because the top 18 airports are fully connected. This network is an example where other randomisation techniques could introduce correlations when generating a null–model network if multiple links between nodes are not allowed [19]. As we

have not put any restrictions in the MAXENT formulation about the number of links that two nodes can share, we use the airport network to show that the MAXENT predicts that on average high degree nodes have more than one link. An example of this is shown in Fig. 3(d) where the number of links between the node with rank 38 and the nodes with ranks 1 to 37 are marked with a solid triangle and the average number of links using Eq. (3) and the MAXENT solution (open circles) and the standard deviation (dashed lines). As expected the null-model predicts that on average two nodes could share more than one link.

The results from the co-authorship and airports networks show that the method to construct surrogates that conserve the rich-club using a preferential attachment [13] (see Eq. (6)) is bias and only works when the degree sequence decays as a power law. The bias is because the surrogates introduce correlations between nodes of low degree. Hence these surrogates are useful when studying correlations between high degree nodes of power law networks.

4.3 Larger networks

Finding the MAXENT solution for medium to large network numerically can be very challenging. However we can use Eq. (26) to approximate $p_{g(i,j)}$ with reasonable accuracy using the following procedure

- measure k_r and $\Delta E(r)$ from the network under consideration,
- propose a function to approximate $T(r, N)$, for example using $s(r) \approx A/(N - r) + B$
- find the values of A and B by minimising $\bar{\eta} = 1/N \sum_r^N ((k_r - \hat{k}_r)/k_r)^2$, where \hat{k}_r is obtained using Eq. (3).

We tested this approach with the word association network [20] which consist of 10,572 nodes and 72,175 links. The fit gave the values of A and B where the average relative error $\bar{\eta} = 1 \times 10^{-4}$. The largest discrepancy between the degree of the network data and the null-model was of two links. Fig. 4(a) shows the average degree-degree correlation of the original data (solid squares) is well approximated by the null-model (open circles). Again we noticed that for low degrees there is a discrepancy between the original network and the null-model suggesting that the null has more links between nodes of low degree with nodes of high degree. To verify if this is the case we evaluated the degree-degree frequency for the links that have at one end a node with degree one, shown in Fig. 4(b). The data shows that nodes of degree one tend to connect with nodes of degree 19. This is also the case for the null-model, where the mode of the distribution is also 19. However, the null also shows a small tendency for nodes of degree one to connect with nodes of higher degree, this tendency is not present on the original network.

5 Concluding Remarks

The main result on the analysis of the MAXENT solution when the rich-club coefficient is conserved is the formula (26), which shows that the linking probabilities between nodes can be described by a specific mass probability function. One of the main advantages of knowing the shape of the mass probability function is that it can be used to approximate the MAXENT solution without resorting to the Lagrangian multipliers method, which generates a large set of non-linear equations which are difficult to solve numerically.

For the networks studied here, the MAXENT ensemble captures the preferential connectivity with nodes of high degree, and as shown in the case of the co-authorship networks, also a

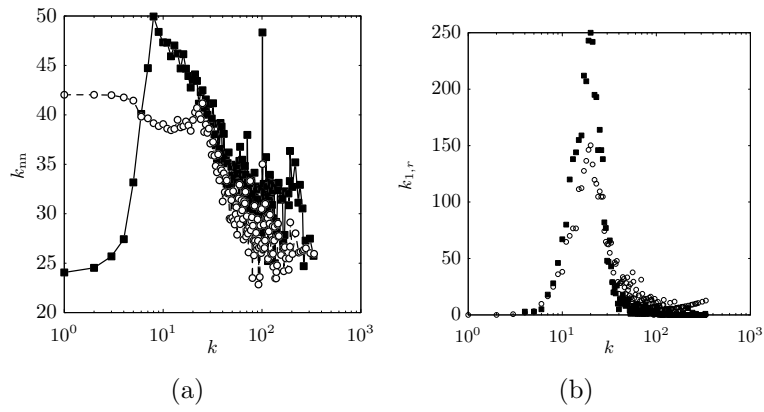


Figure 4: Word Association Network. (a) Comparison of the average degree–degree correlation obtained from the data (filled squares) and the one obtained from the approximation of the MAXENT solution (open circles). (b) Degree–degree frequency of the links with a node of degree one at one end where the network data is shown with filled squares and the null–model with open circles.

preferential linking between nodes of low degree. As the method does not put restrictions on the number of links that two nodes can share, it can be used to analyse networks that have a densely connected rich–club. The method gives a good approximation to the average degree–degree distribution but it is more general, as it can describe in more detail the connectivity between nodes with different degree, as it was shown in the case of the word association network.

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